

Microstructural Simulations of Texture-Induced Physical Behavior

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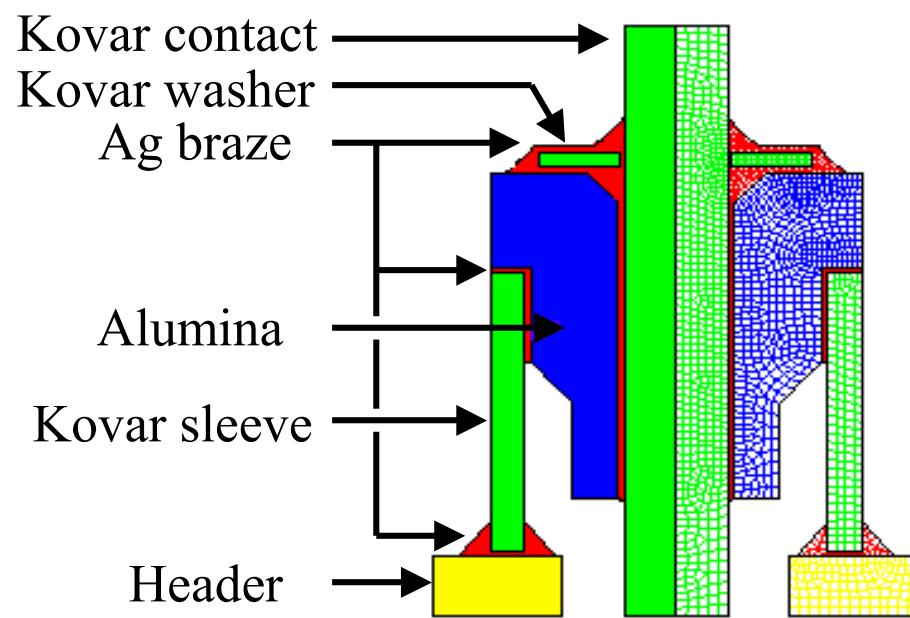
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105th Annual Meeting of ACers
"Microstructure Evolution and Control"
Opryland, TN — April 29, 2003

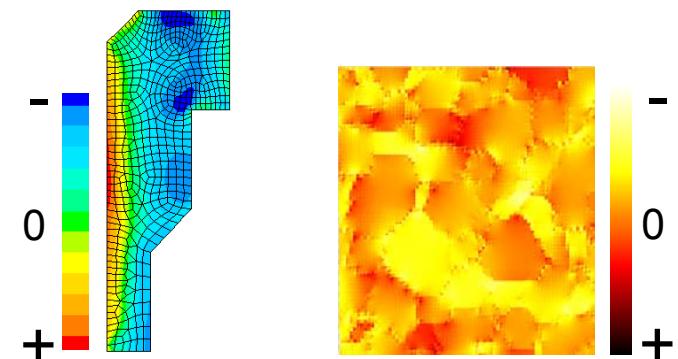
Predict Reliability of Ceramic-Containing Components



Residual Stresses due to:

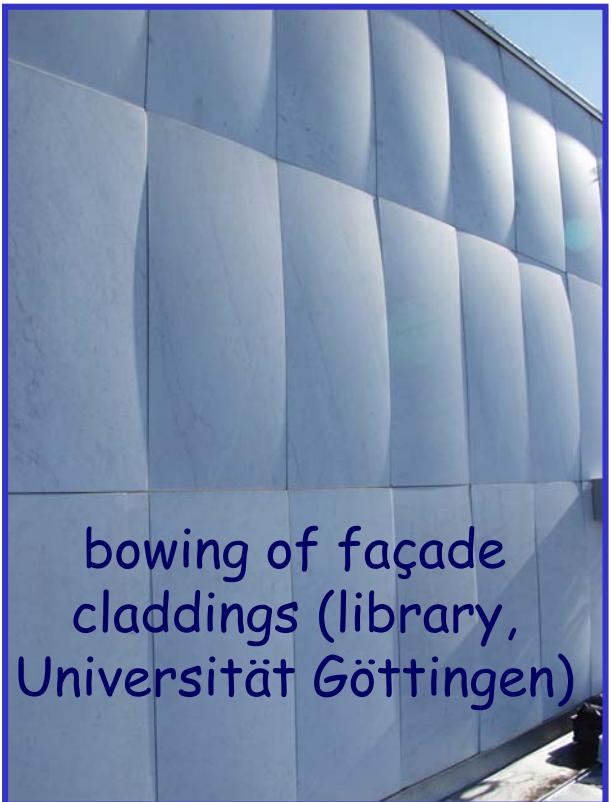
thermal
expansion
mismatch

thermal
expansion
anisotropy

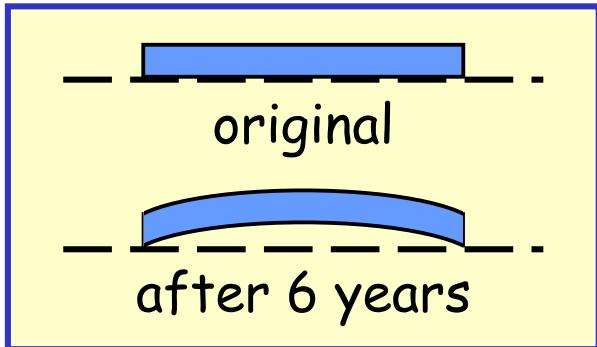
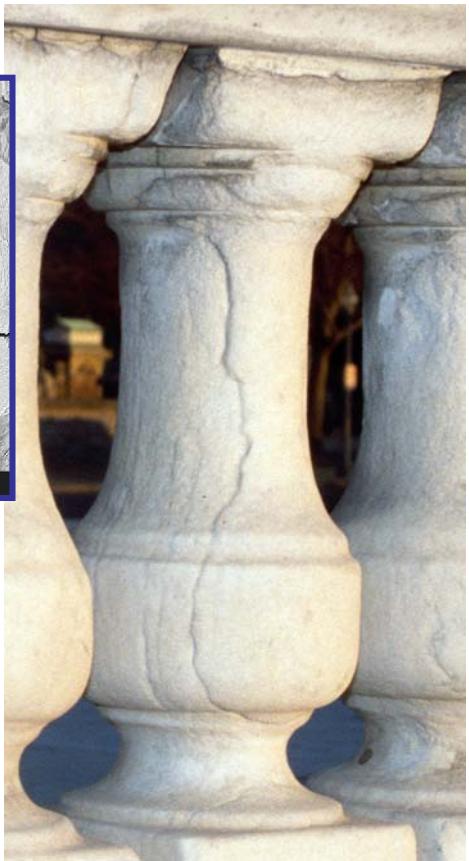
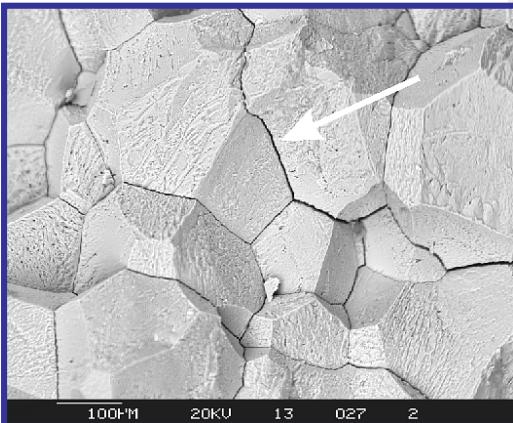


residual stresses can cause spontaneous microcracking and influence R-curve behavior & crack propagation under applied loads

Venkata R. Vedula, Shekhar Kamat & S. Jill Glass, Sandia National Laboratories



Elucidate Thermal Degradation of Marbles

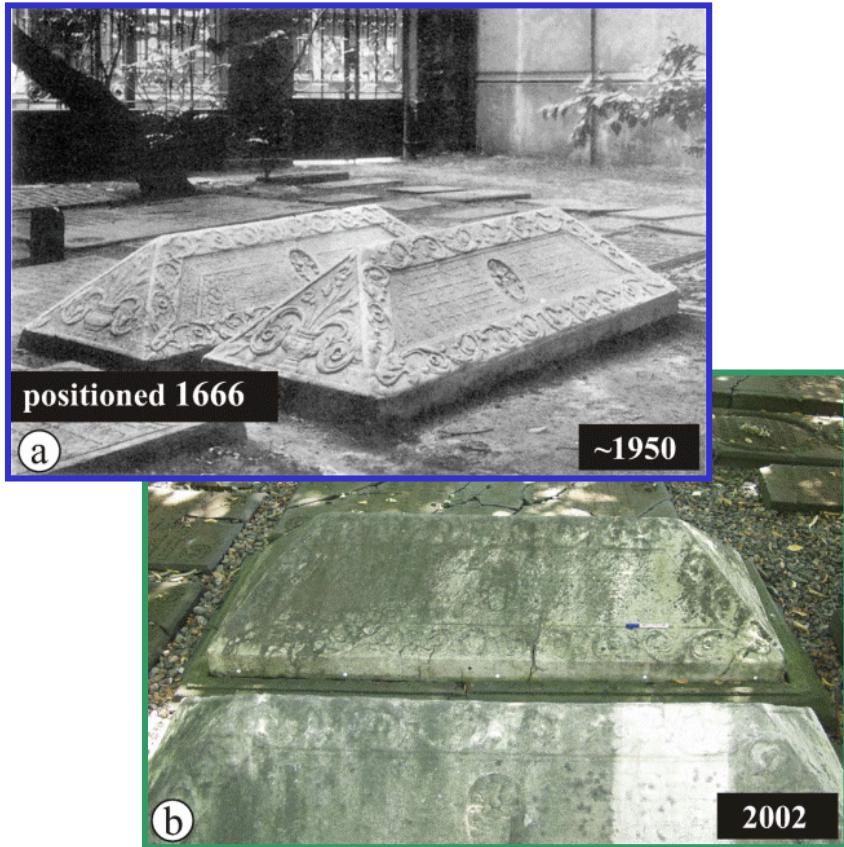


granular
disintegration

Thomas Weiß and Siegfried Siegesmund, Universität Göttingen, Germany

Preservation of Antiquity Artifacts

Jewish cemetery in Hamburg
Altona (marble tombstones)



Siegfried Siegesmund, Thomas Weiß & Joerg Ruedrich, Universität Göttingen, Germany



Getty Conservation Institute
museum, Los Angeles

Texture-Induced Physical Behavior

Objective: *elucidate the influence of various types of texture on the ensemble physical properties and behavior of polycrystalline ceramics*

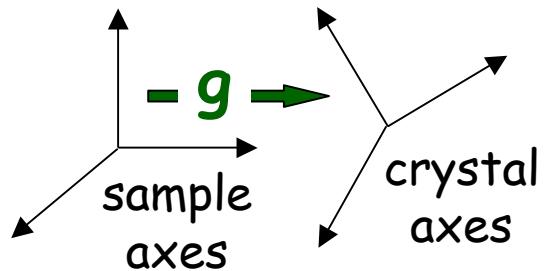
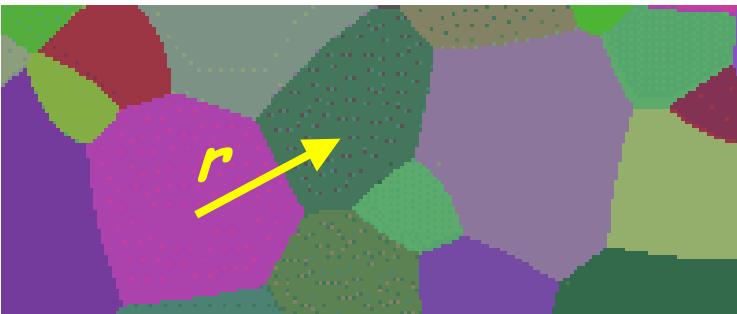
Contents:

- Statistical Description of Texture
 - Statistical description of microstructure
 - Types of texture
- Microstructural Simulations
 - TEA induced residual stresses
 - Ensemble physical properties, e.g., elastic energy density and coefficient of thermal expansion

Statistical Description of Microstructure

Microstructure Descriptor: $h = \{c, \phi, g, \dots\}$

- composition: c
- phase: ϕ
- crystal orientation: $g = \{\varphi_1, \Phi, \varphi_2\}$



Microstructure Statistics

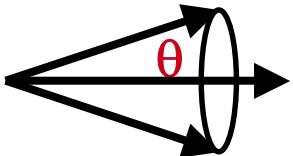
- 1-point statistics: $f_1(h)$
- 2-point statistics: $f_2(h, h' | r)$

Grain-Boundary Statistics: $S(\Delta g, n)$

adapted from
Surya R Kalidindi

Types of Texture

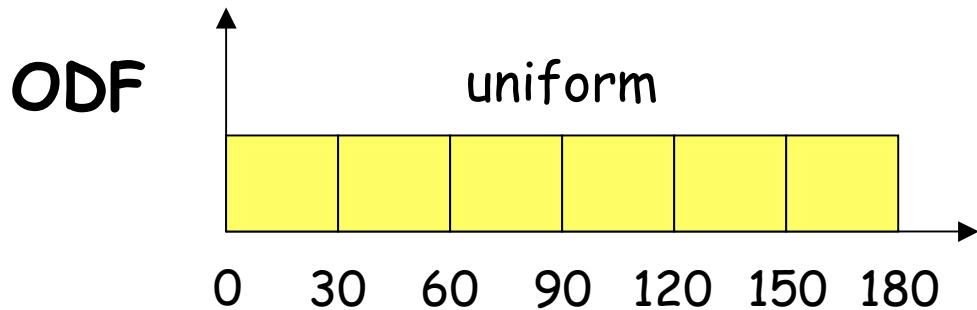
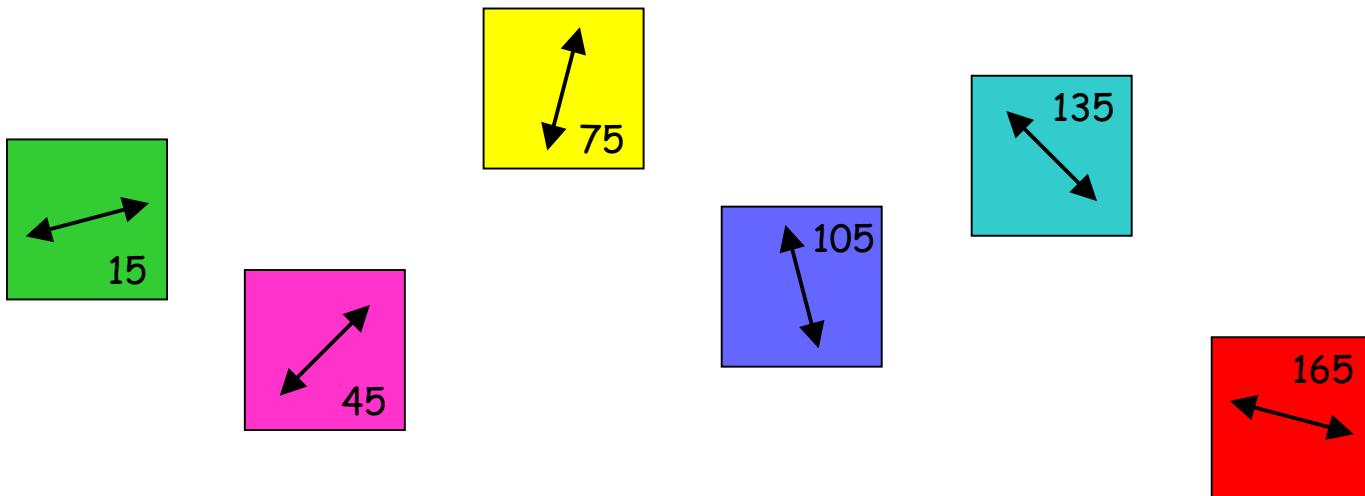
- **Crystallographic Texture**
 - Orientation Distributions Functions (ODF) of grains: $g = \{\varphi_1, \Phi, \varphi_2\}$
 - Random in Euler Space (uniform) $\varphi_1 \in [0, 2\pi]$
 - March-Dollase Fiber Texture $\cos[\Phi] \in [-1, 1]$
 - Others ODF's $\varphi_2 \in [0, 2\pi]$
 - Intercrystalline Misorientation Distributions Functions (MDF): uniform and *high & low*
 - Orientation Correlation Functions (k-point statistics)
- **Grain-Shape Morphologic Texture**



$$f(M, \theta) = M / [\cos^2(\theta) + M \sin^2(\theta)]^{3/2}$$

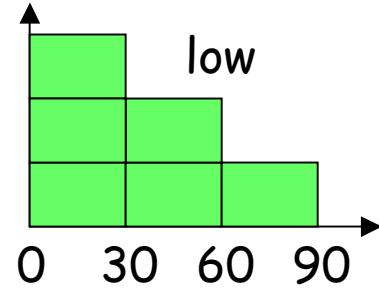
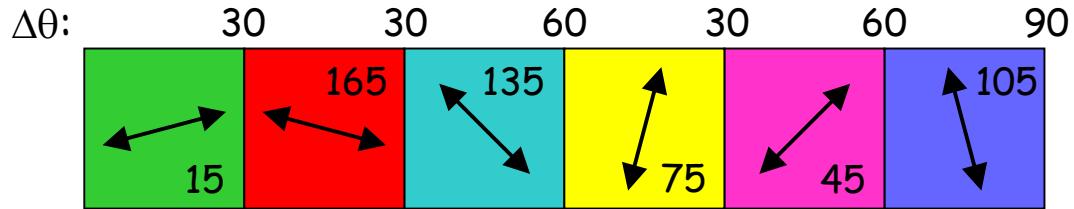
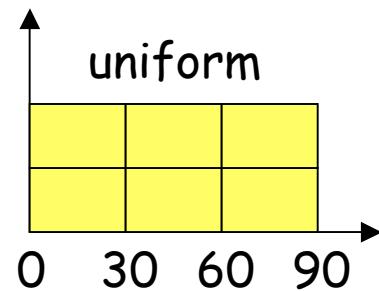
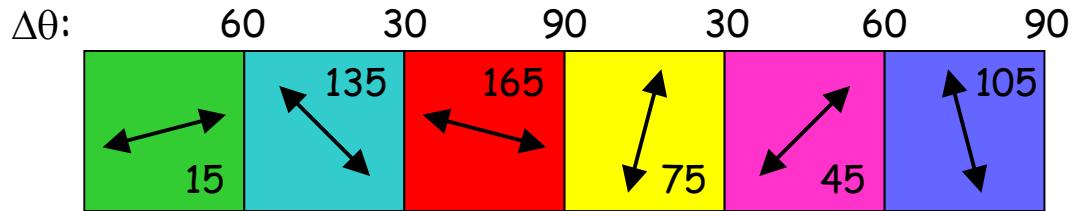
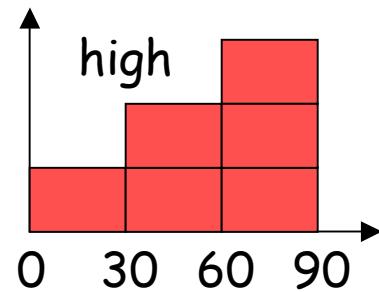
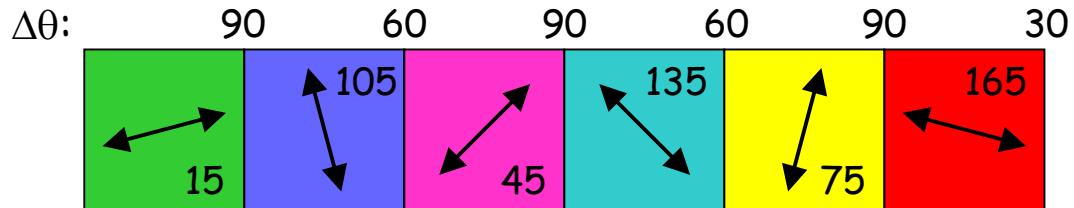
M: max. MRD

Uniform Crystallographic Texture



Types of Misorientation Texture

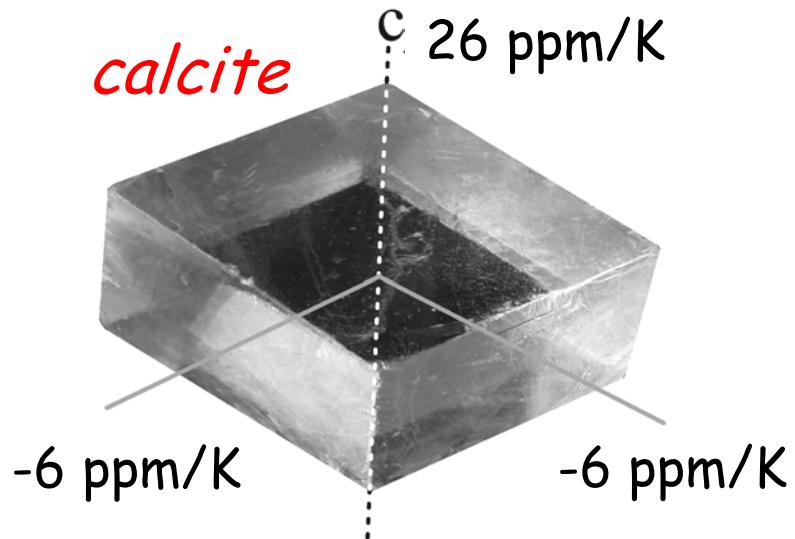
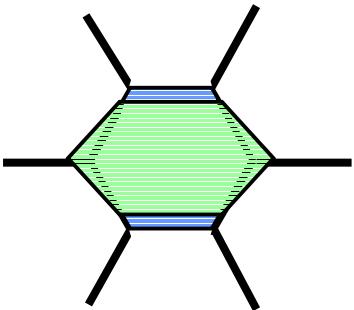
MDF



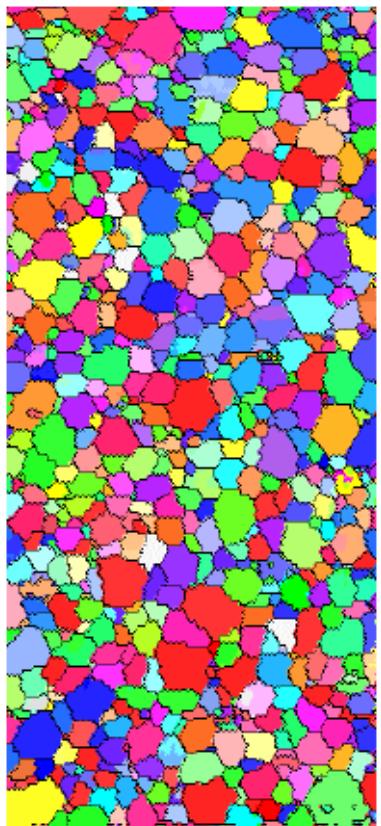
Microstructural Simulations

Crystalline Thermal Expansion Anisotropic (TEA) causes:

- residual stresses between adjacent grains upon heating or cooling



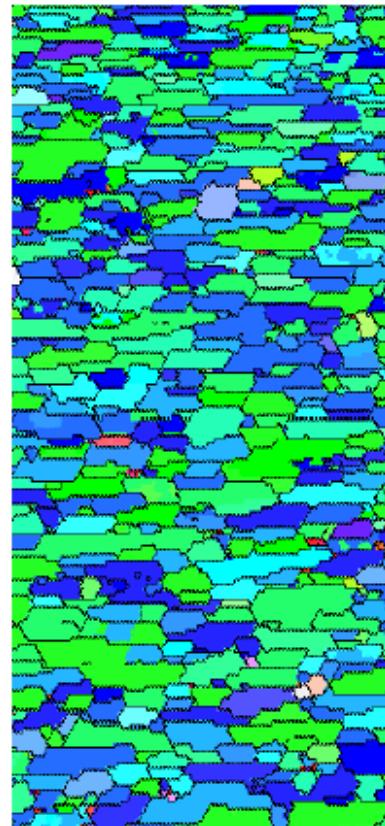
Alumina Microstructure via EBSD



Untextured
(MRD=2)



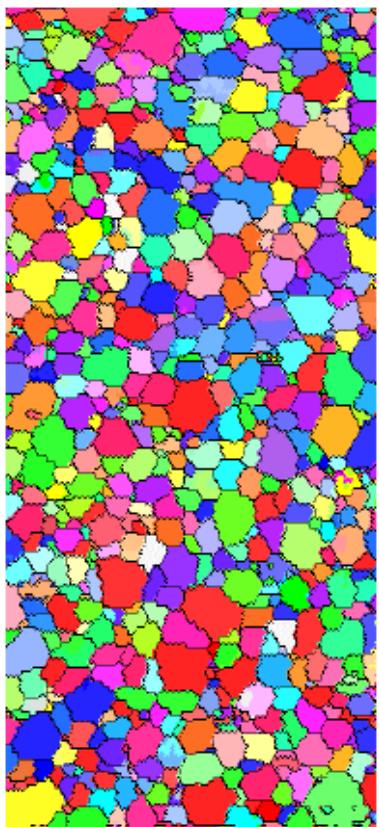
Grain Normals



Textured
(MRD=90)

V.R. Vedula, S.J. Glass, D.M. Saylor, G.S. Rohrer, W.C. Carter, S.A. Langer, and E.R. Fuller, Jr., J. Am. Ceram. Soc., **84** [12], 2947-2954 (2001).

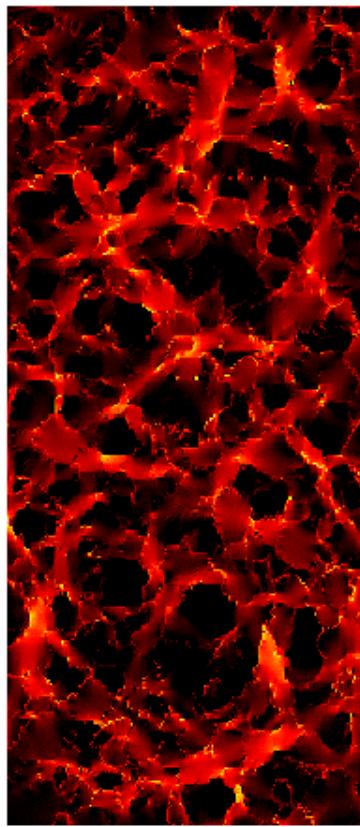
Residual Stress Distribution in Untextured Alumina ($\Delta T = -1500^{\circ}\text{C}$)



EBSD
microstructure



[$\sigma_{xx} + \sigma_{yy}$]
(MPa)

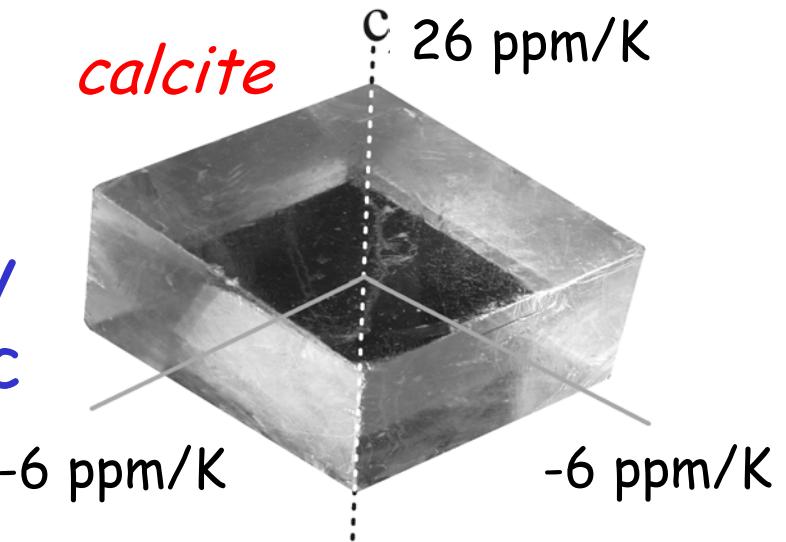


Max. Principal
Stress (MPa)

Microstructural Simulations

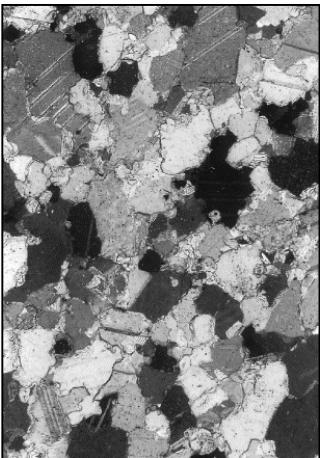
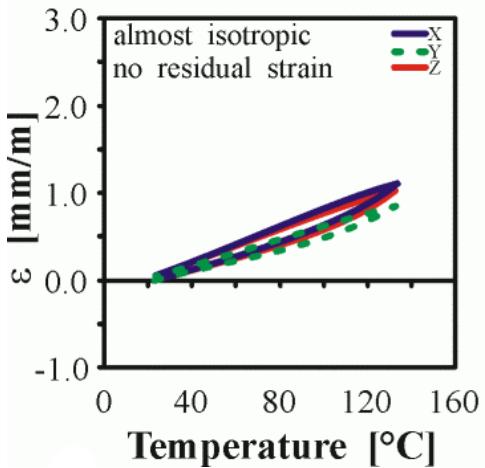
Crystalline Thermal Expansion Anisotropic (TEA) causes:

- residual stresses between adjacent grains upon heating or cooling
- microcracking propensity (characterized by elastic strain energy density)
- anisotropy in bulk thermal expansion

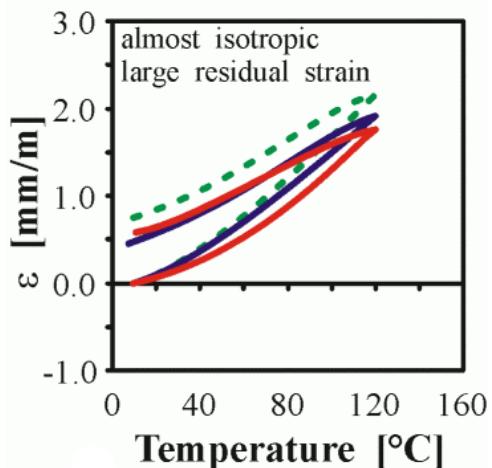


all phenomena are influenced by texture

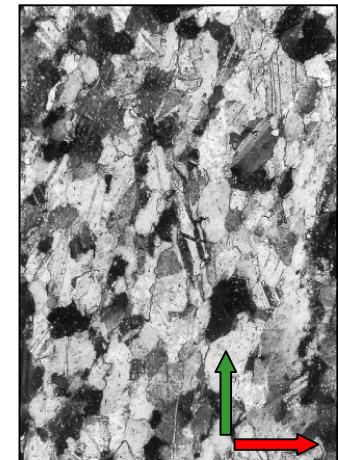
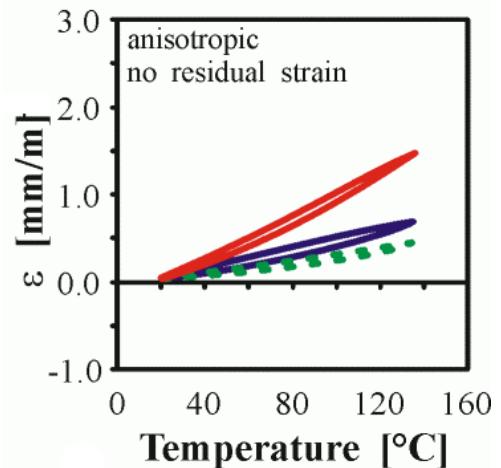
Types of Thermal Expansion



Carrara (Italy)

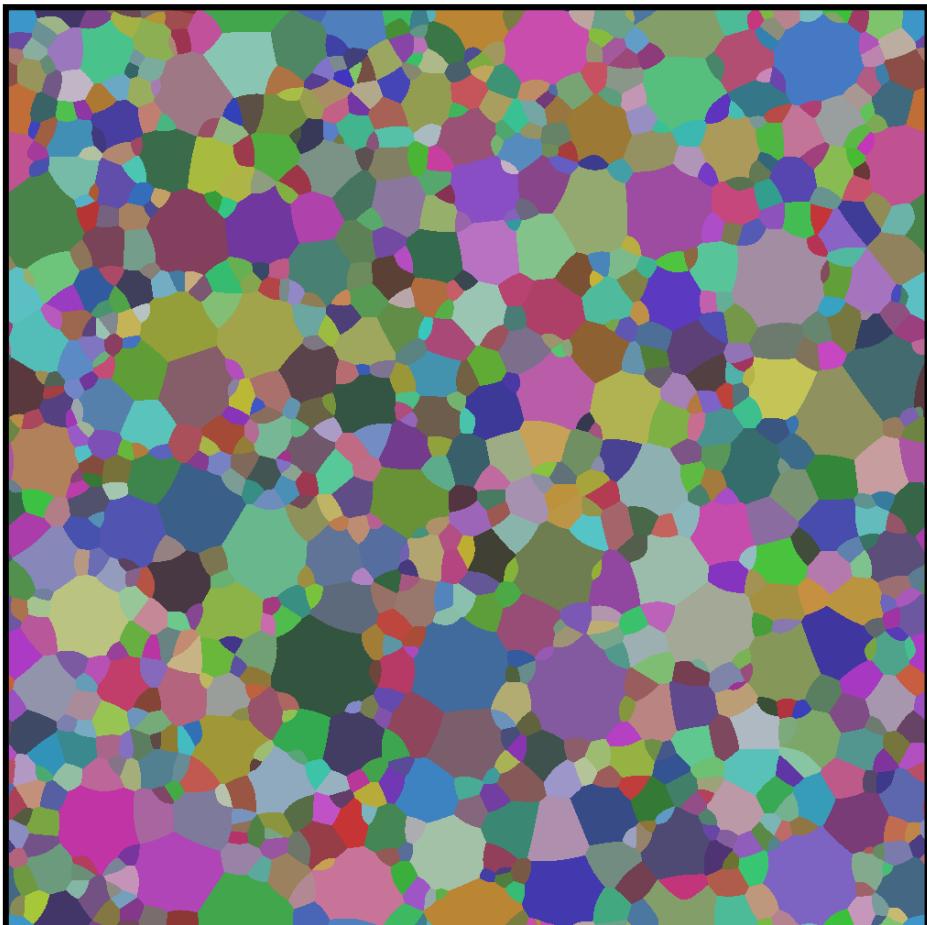


Carrara (Italy)



Kauffung (Poland)

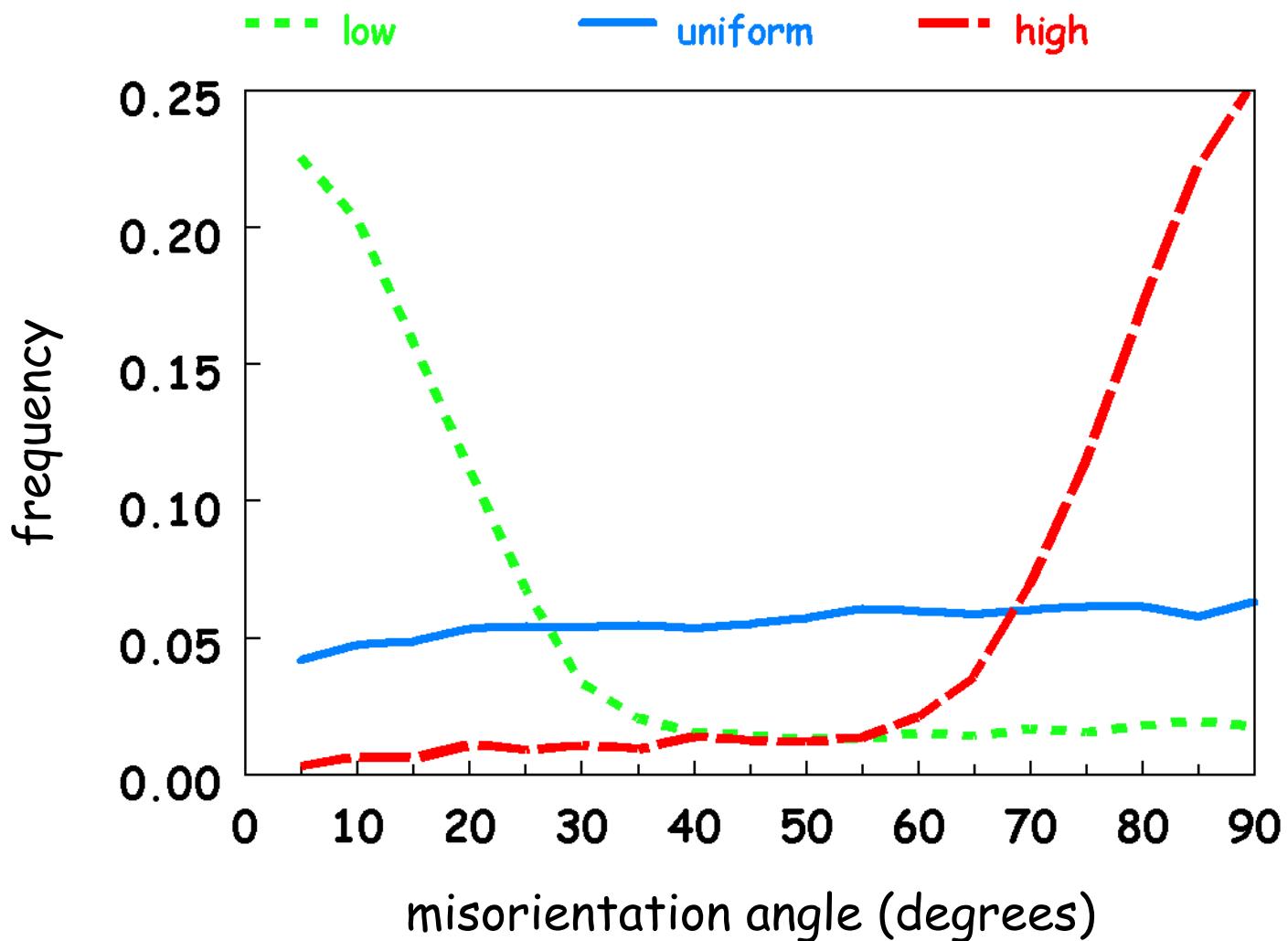
Simulation Model: Microstructure of 924 Grains



Characterized by:

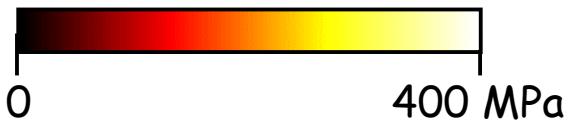
- the same composition: calcite, dolomite, or alumina
- the same thermoelastic properties
- different crystallographic orientations of the grains
- random distribution of grain orientations (i.e., c-axis)
- uniform, and high & low intergranular misorientation distributions

Intergranular Misorientation Distribution Functions

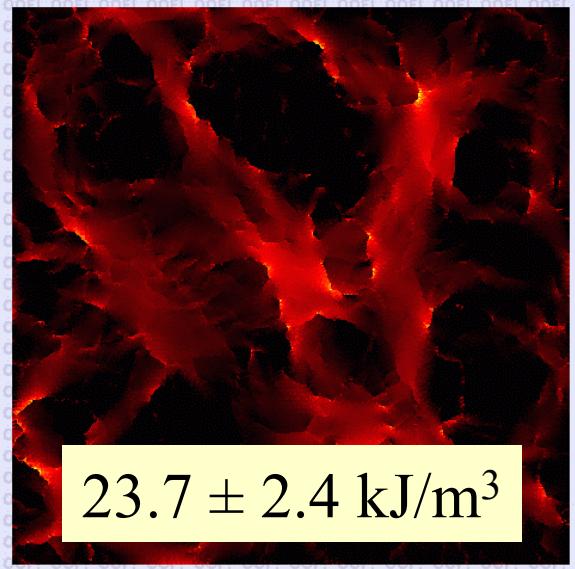


Influence of Grain Misorientation Distribution Function

maximum principal stress for a random grain orientation distribution function

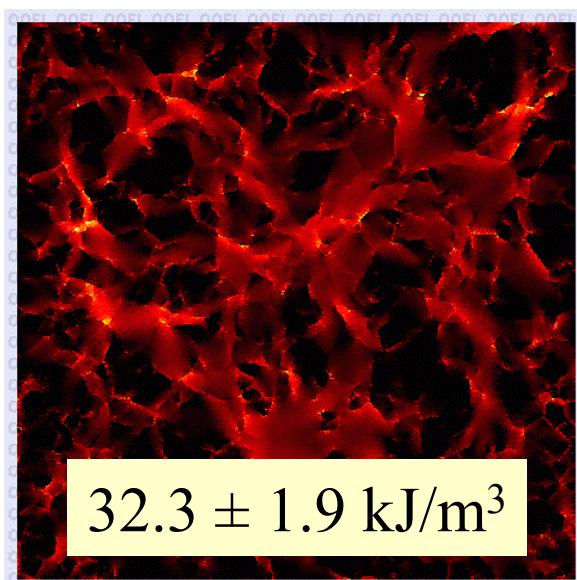


low-angle GB's

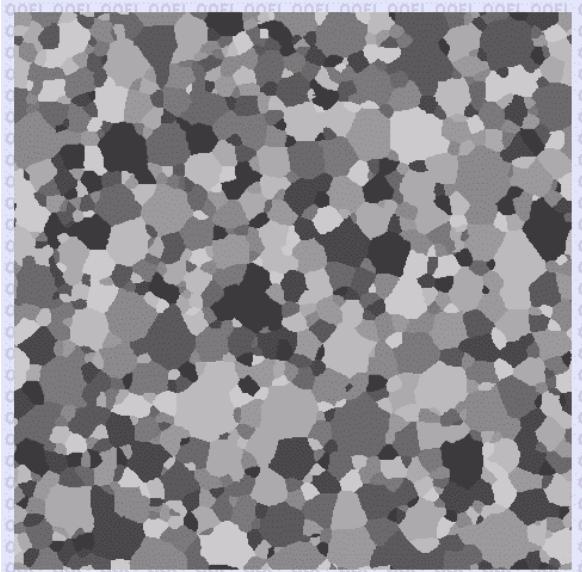


$23.7 \pm 2.4 \text{ kJ/m}^3$

uniform



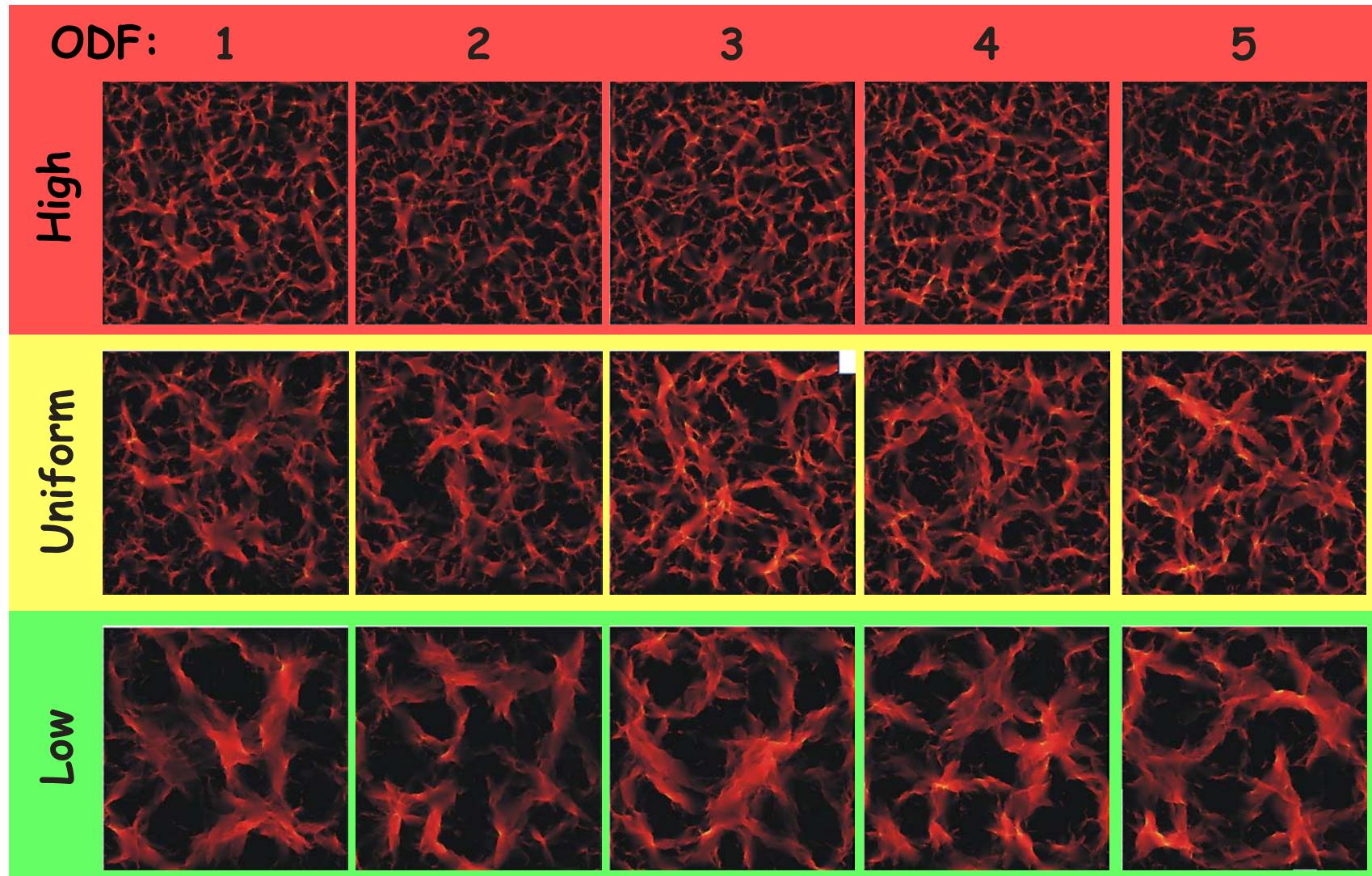
$32.3 \pm 1.9 \text{ kJ/m}^3$



$35.3 \pm 1.0 \text{ kJ/m}^3$

high-angle GB's

Calcite Results



MDF

Maximum Principal Stress upon heating +100°C
for 5 random orientation distributions of *calcite* grains

Alumina Results

ODF: 1

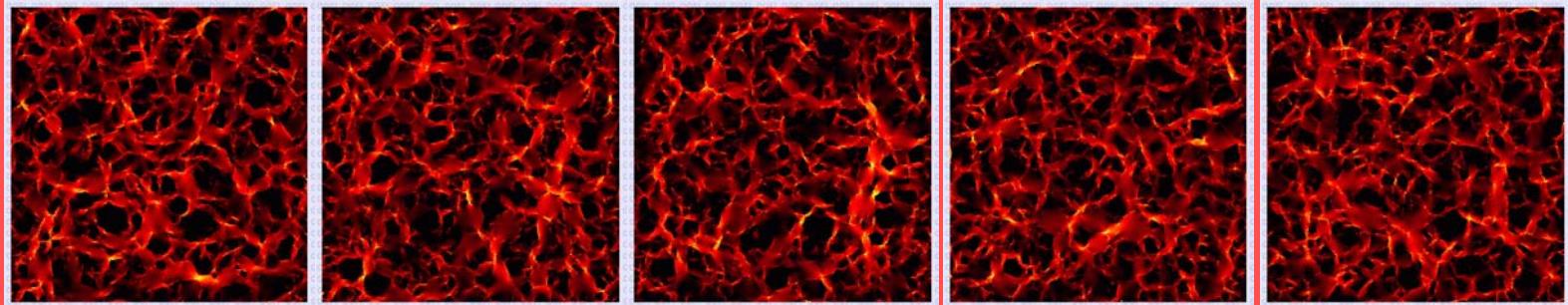
2

3

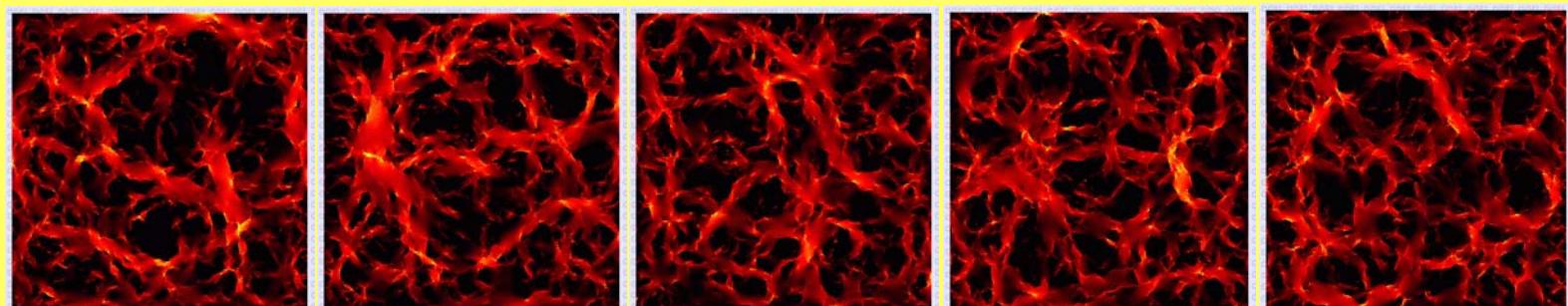
4

5

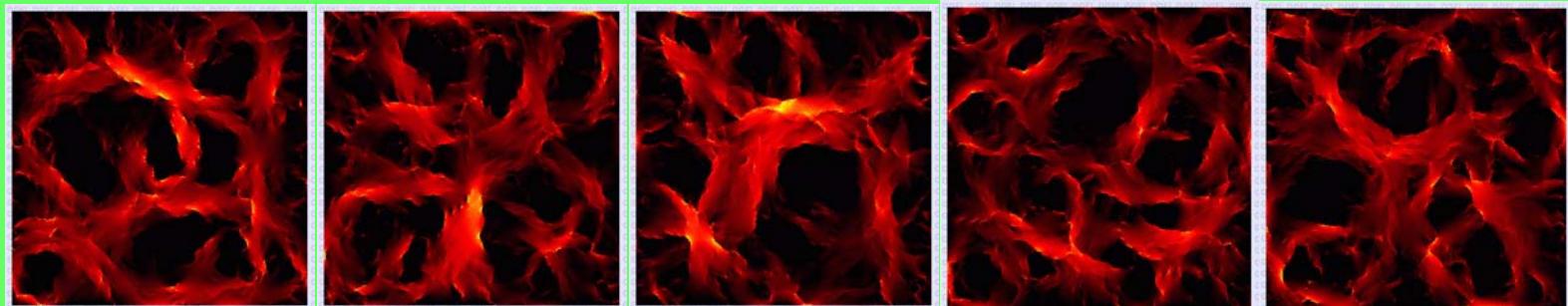
High



Uniform



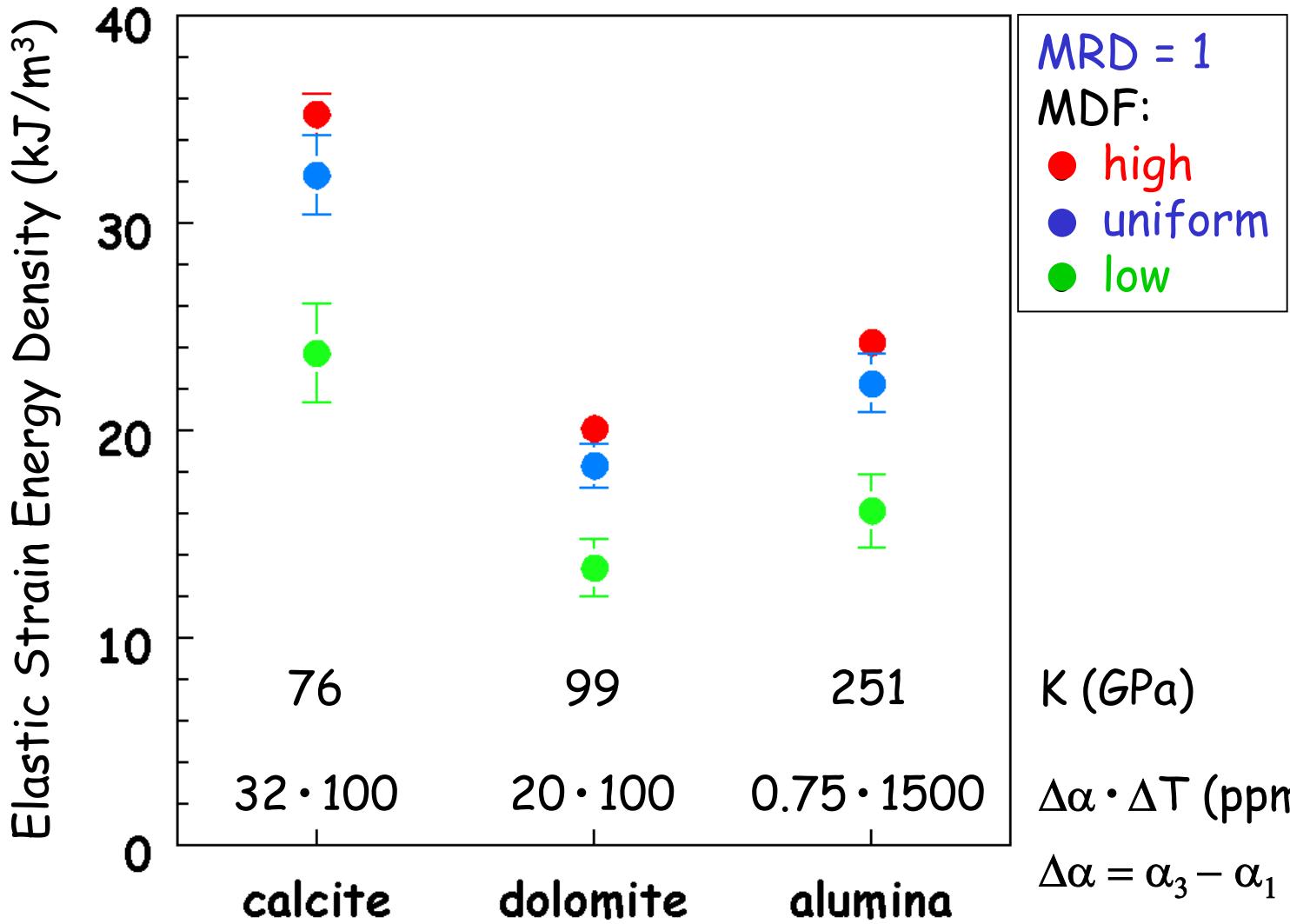
Low



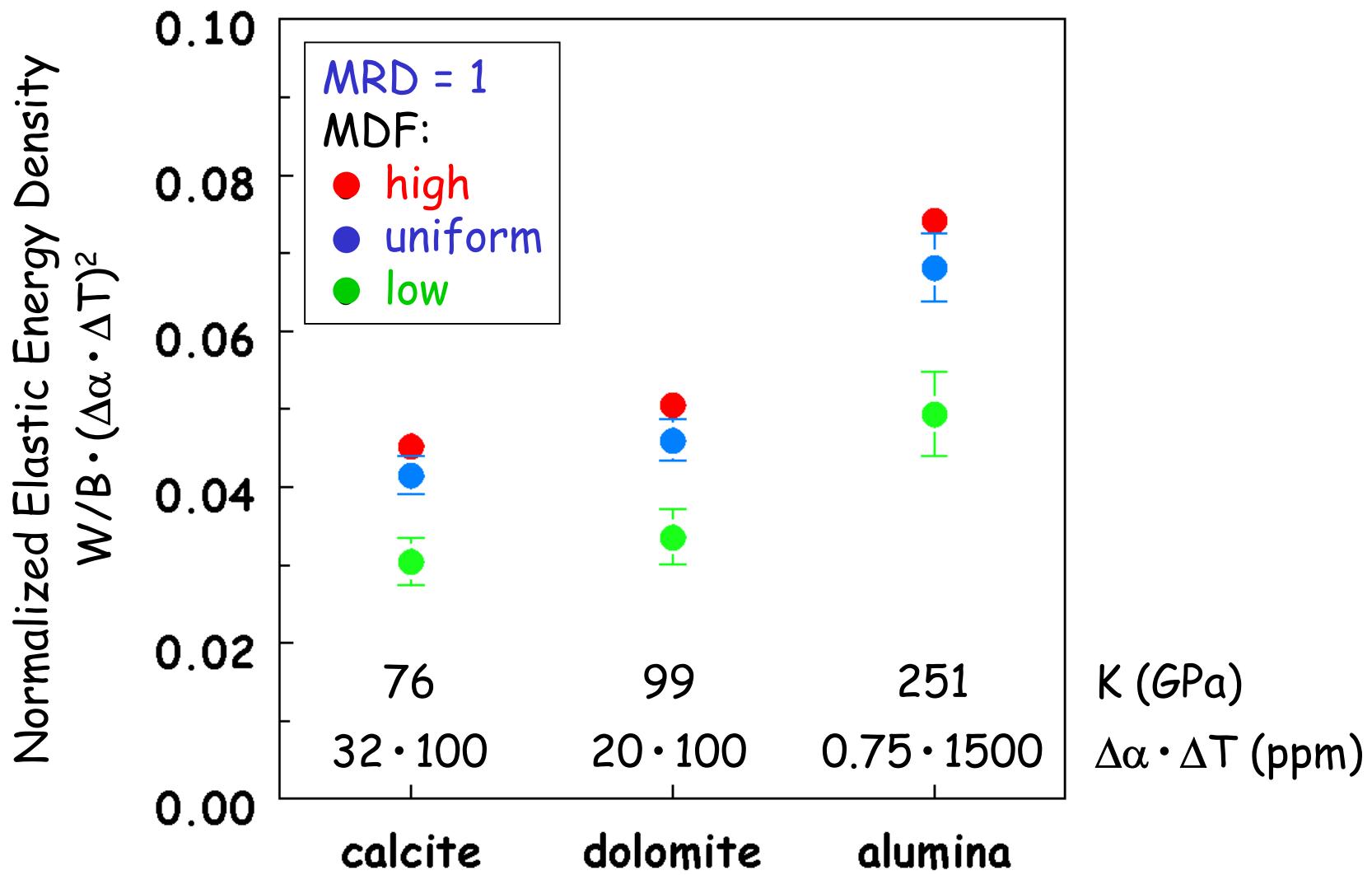
MDF

Maximum Principal Stress upon cooling - 1500°C for 5 random ODF's orientation distributions of *alumina* grains

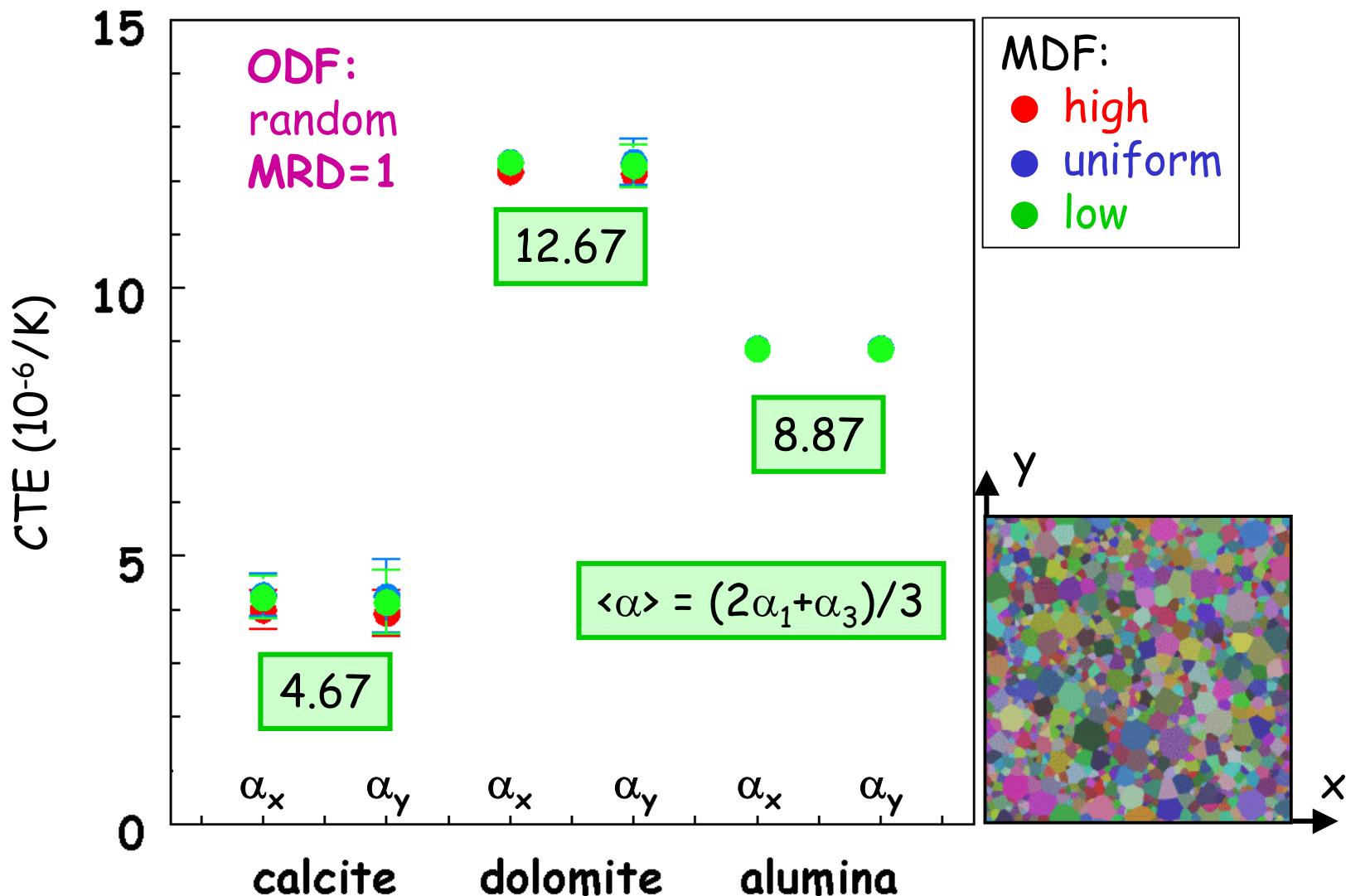
Elastic Strain Energy Density



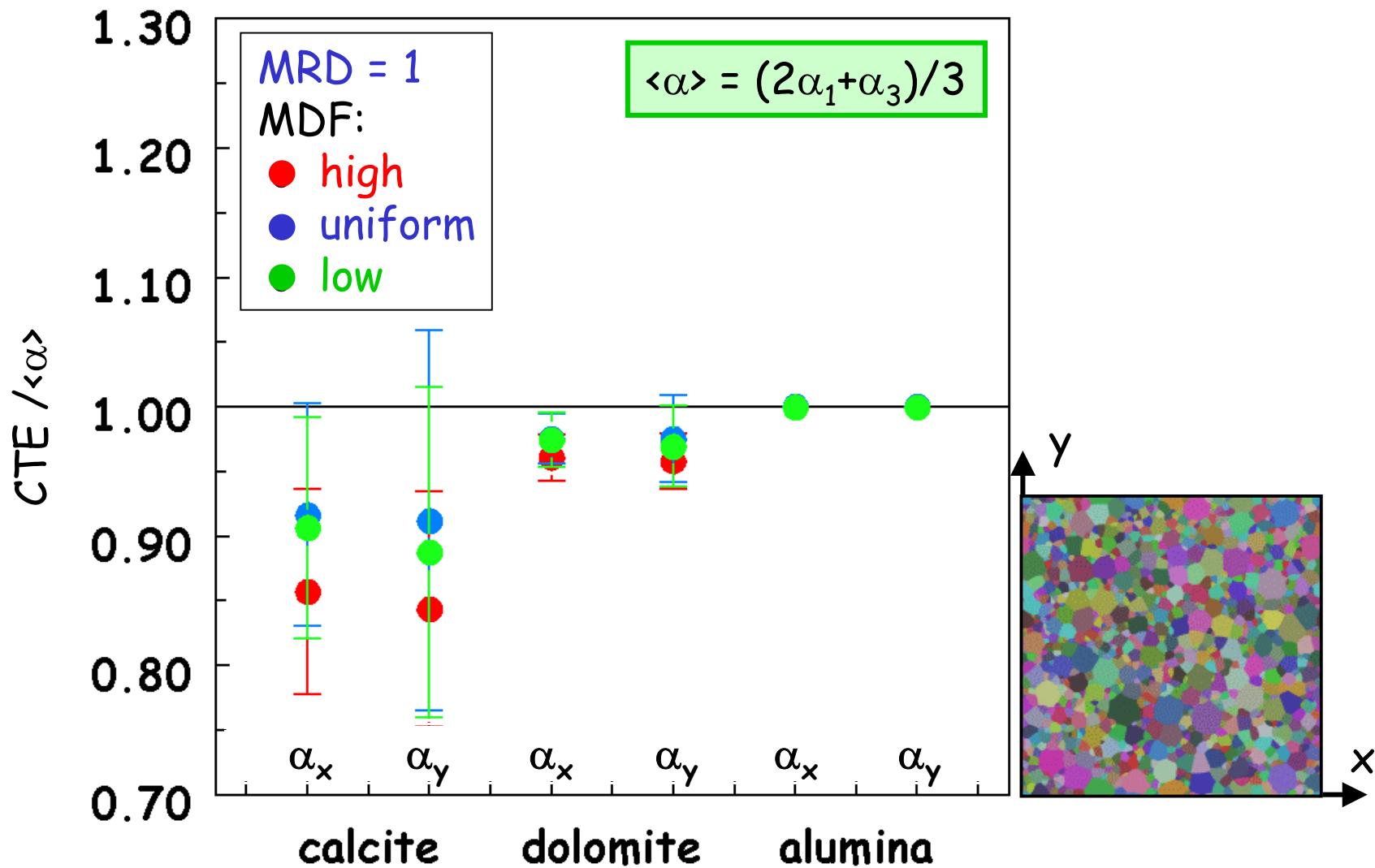
Normalized Elastic Energy Density



Bulk Coefficient of Thermal Expansion

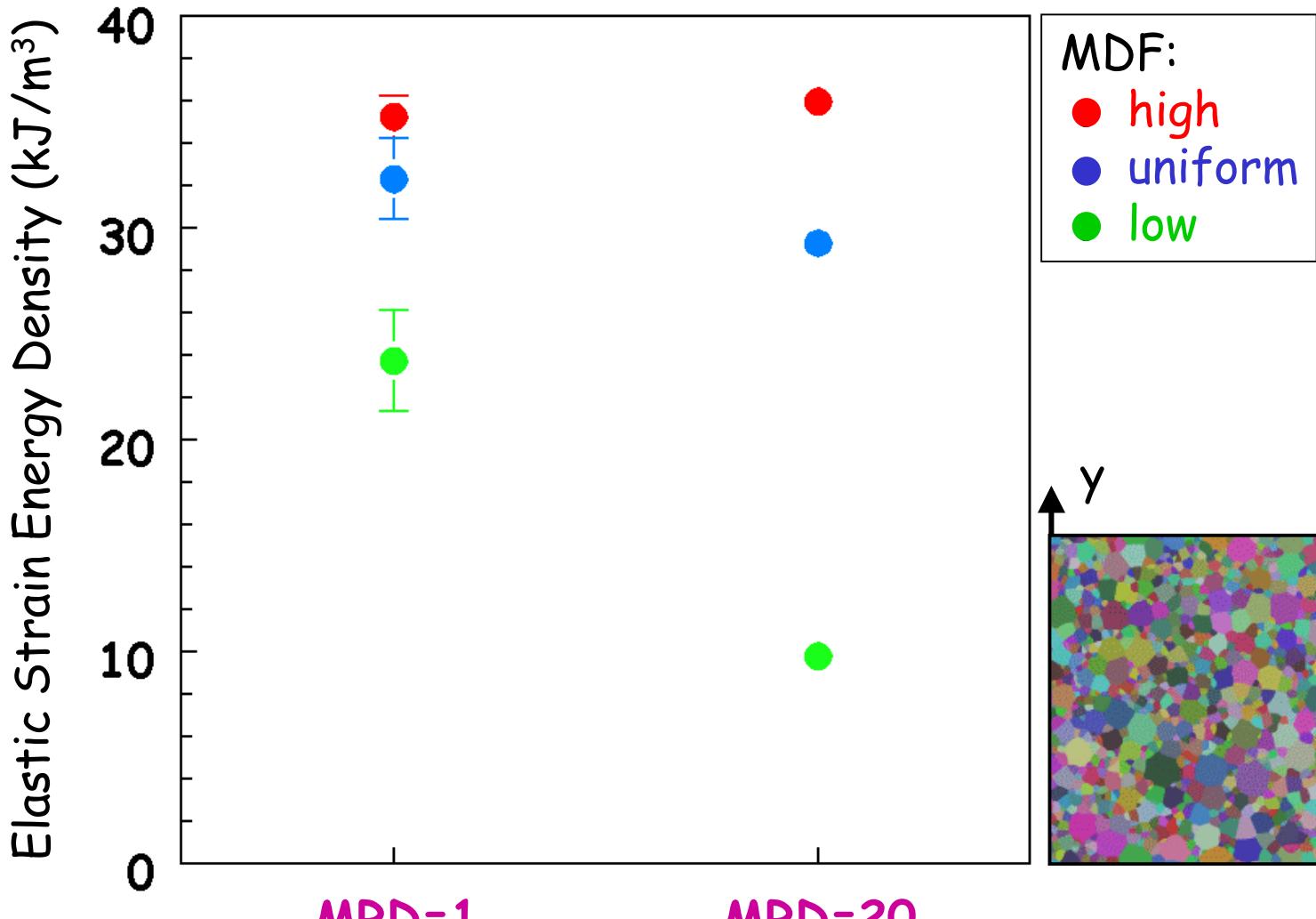


Normalized Bulk CTE

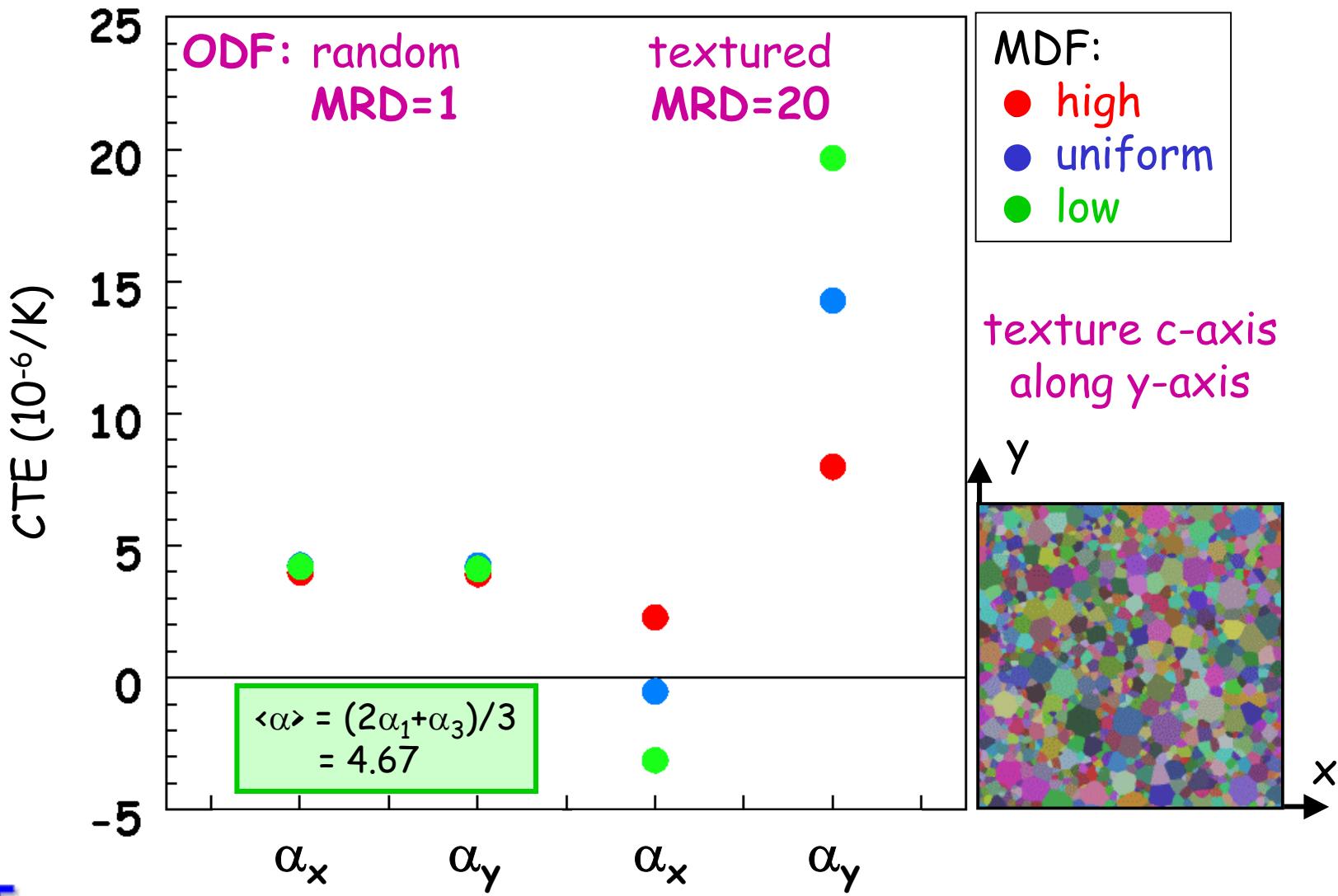


Elastic Strain Energy Density

for calcite heated +100°C

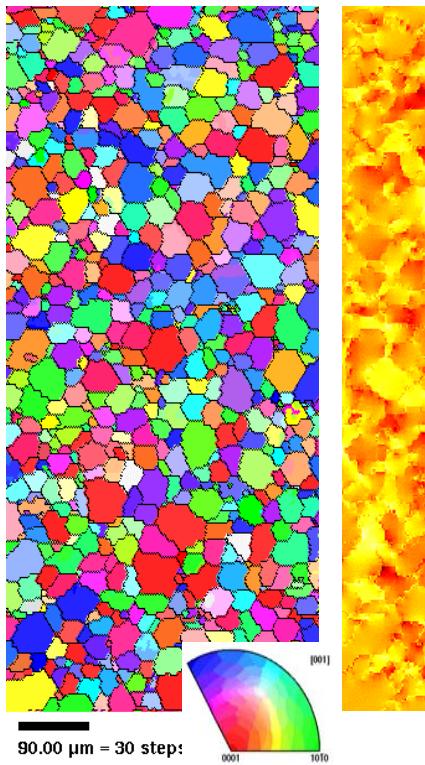


Bulk Coefficient of Thermal Expansion for calcite heated +100°C

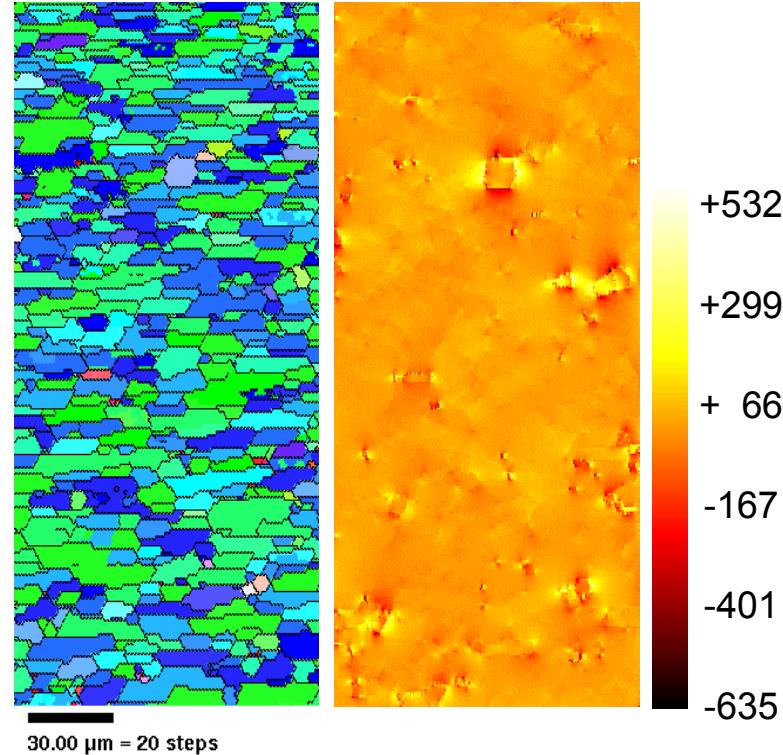


Residual Stresses in Textured Alumina

Untextured (MRD=2)



Textured (MRD=90)



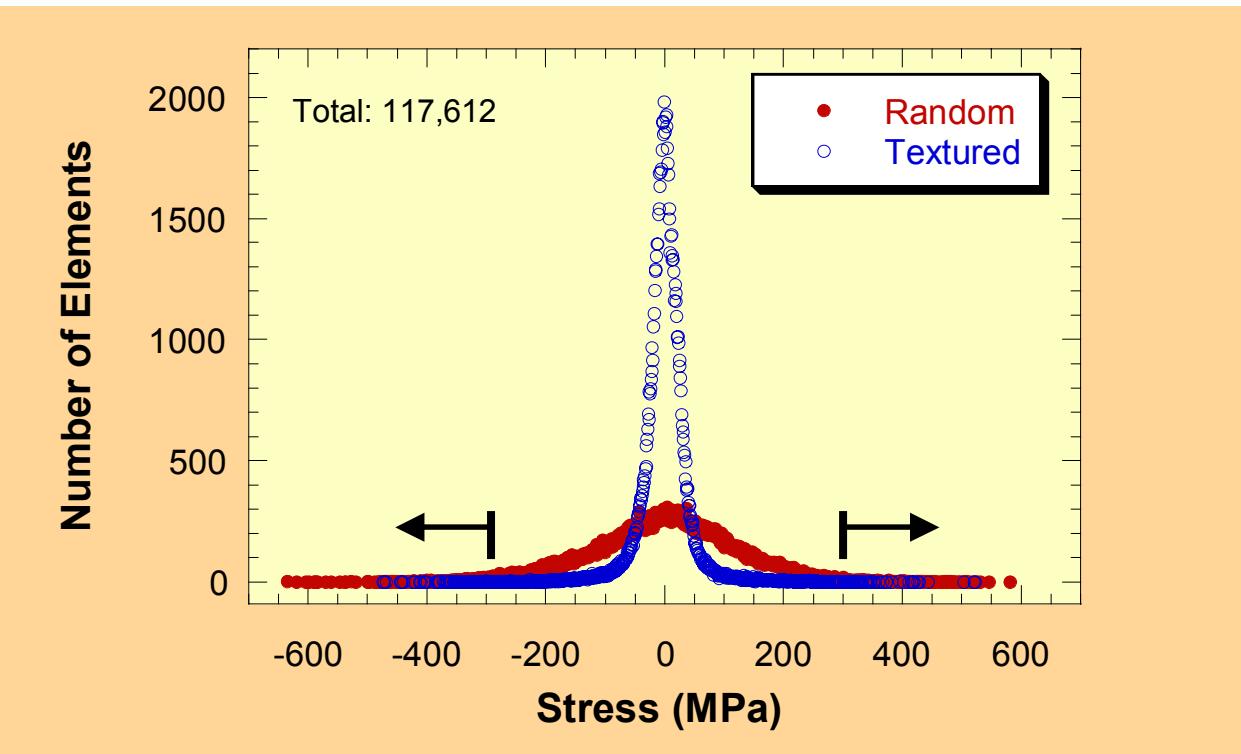
Stress Invariant ($\sigma_{11} + \sigma_{22}$) for $\Delta T = -1500^\circ\text{C}$

plane stress with free boundary conditions — total number of elements = 117,612

Venkata R. Vedula, Edwin R. Fuller, Jr., and S. Jill Glass

Materials Science & Engineering Laboratory

Residual Stress Distributions

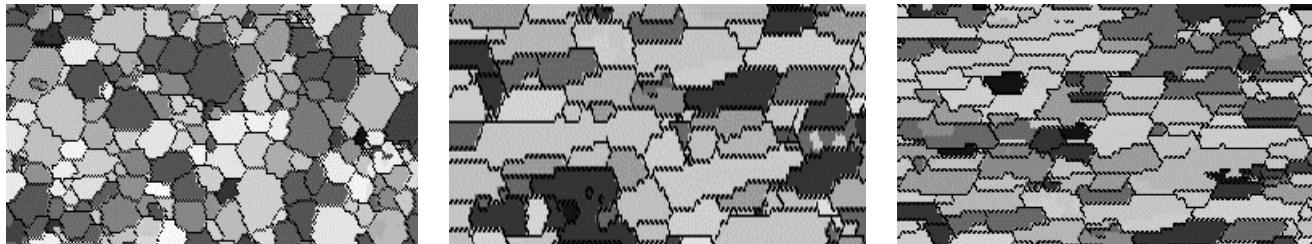


of Elements with $|\sigma_{11} + \sigma_{22}| > 300$ MPa

Random = 2563 ($\approx 2.2\%$)

Textured = 221 ($\approx 0.2\%$)

Morphologic versus Crystallographic Texture in Alumina



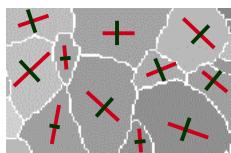
Aspect Ratio:

1:1

4:1

8:1

MRD:

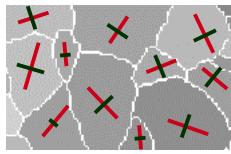


1

A1

B1

C1

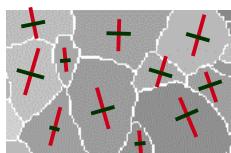


40

A40

B40

C40



100

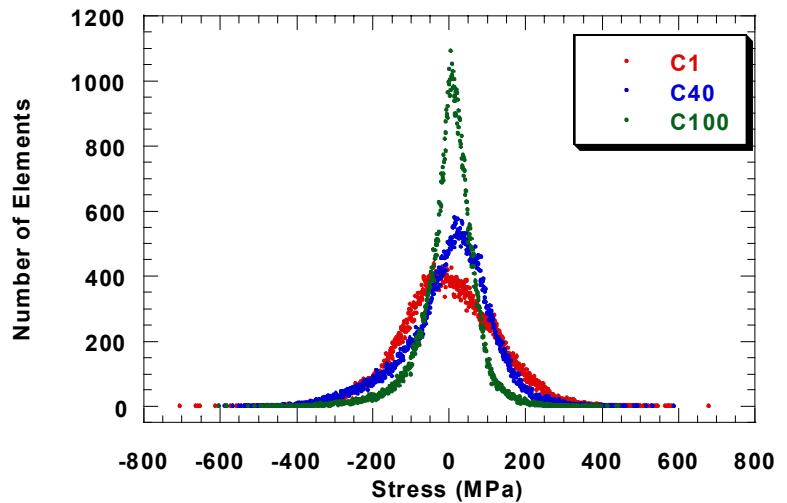
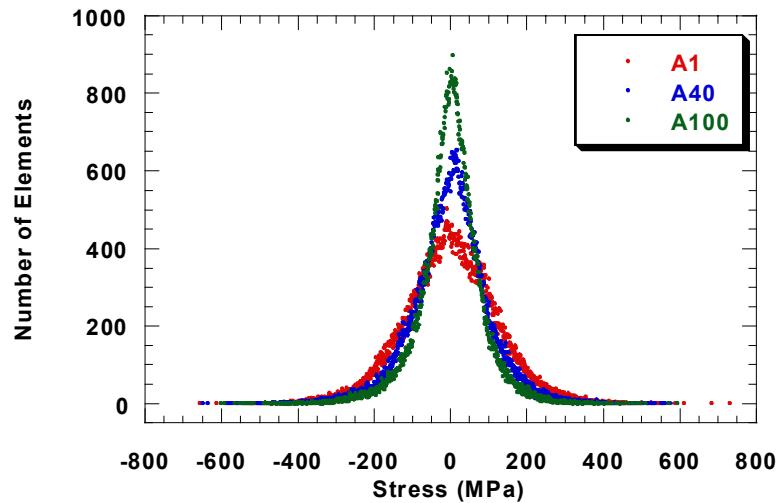
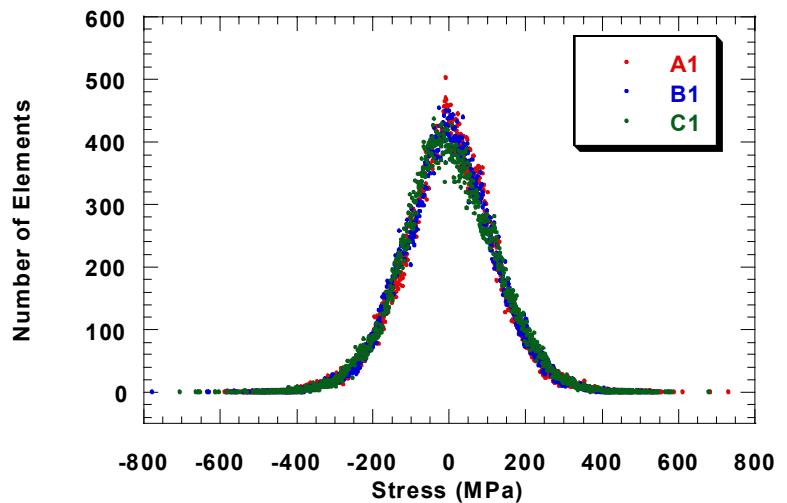
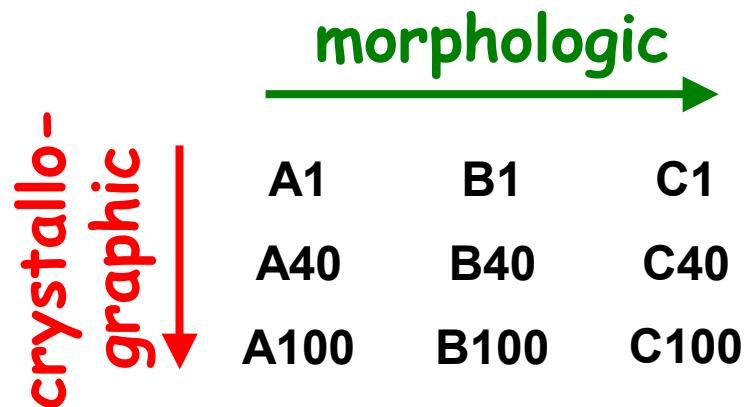
A100

B100

C100

Experimental Microstructures

Residual Stress Distributions



Texture-Induced Physical Behavior

SUMMARY:

- Both crystalline orientation texture and intercrystalline misorientation texture significantly influence TEA residual stresses and microcracking propensity (via average elastic energy density)
- Intercrystalline misorientation texture gives rise to TEA residual stress networks in the microstructure
 - ➡ network size (with respect to grain size) depends on the MDF
- Together crystal orientation texture & intergranular misorientation texture determine average thermal expansion behavior (coefficients & their anisotropy)
- Grain-shape morphological texture appears to have a minor influence on TEA residual stresses

Abstract

Microstructural Simulations of Texture-Induced Physical Behavior

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37077 Göttingen, Germany

Due to anisotropy crystalline properties, texture can have a profound influence on ensemble physical properties and behavior of polycrystalline ceramics. Microstructure-based finite element simulations are used to elucidate the influence of texture on polycrystalline physical properties, such as elastic moduli and coefficients of thermal expansion, and on physical behavior, such as residual stresses and microcracking propensity. Both real and simulated microstructures are considered. Real microstructures include untextured and textured alumina, and natural dolomite marble. Simulated microstructures are generated via either Monte Carlo grain-growth algorithms or an anisotropic reconstructed algorithm, which can generate morphological as well as crystalline texture. Influences of several types of crystallographic texture are considered: grain orientation distributions, grain misorientation distributions, grain-boundary planes distributions, and orientation correlation functions.